Real-Space Renormalization Group Study of the Anisotropic Antiferromagnetic Heisenberg Model on the Square Lattice *

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In this work we apply two different real-space renormalization-group (RSRG) approaches to the anisotropic antiferromagnetic spin-1/2 Heisenberg model on the square lattice. Our calculations allow for an approximate evaluation of the T vs. Δ phase-diagram: the results suggest the existence of a critical value of $\Delta > 0$, at which the critical temperature goes to zero, and the presence of reentrant behavior on the critical line between the ordered and disordered phases. This whole critical line is found to belong to the same universality class as the Ising model. Our results are in accordance with previous RSRG approaches but not with numerical simulations and spin-wave calculations.

I. INTRODUCTION

Two-dimensional antiferromagnetism plays an important role in the description of La_2CuO_4-based high-temperature superconductors [1]. In these, the spin fluctuations in the CuO_2 planes are well described by the spin-1/2 antiferromagnetic Heisenberg model on a square lattice. This, together with the theoretical discussion made by Anderson [2], has raised the interest on this model, which has been a challenge for decades.

The Hamiltonian of the anisotropic Heisenberg model reads:

$$- \beta \mathcal{H} = K \sum_{\langle i,j \rangle} \left[(1 - \Delta) \left(S_i^x S_j^x + S_i^y S_j^y \right) + S_i^z S_j^z \right], \quad (1)$$

where $K = J/kT$ is the dimensionless exchange parameter, with $K < 0 (> 0)$ for the antiferromagnetic (ferromagnetic) model, k is the Boltzmann constant, T is the temperature, the sum is over pairs of nearest-neighbor spins i and j, S_l^λ is the λth component of the spin-1/2 Pauli operator on site l, Δ is the anisotropy parameter, and $\beta = 1/kT$. Note that $\Delta = 0$ describes the isotropic Heisenberg model and for $\Delta = 1$ we regain the Ising model.

For $J > 0$ (ferromagnetic interactions), the ground state is well known and the Mermin-Wagner theorem excludes long-range order at finite temperatures in two dimensions for $\Delta = 0$ [3]. On the other hand, for $0 < \Delta \le 1$ there is an easy-axis and the symmetry is the same as for the Ising model; therefore, long-range order is possible. Indeed, the universality class for all models with values of $\Delta \ne 0$ is the same as for the Ising model. A schematic temperature vs. anisotropy phase-diagram for the ferromagnetic model is presented in Fig.1, where all the features discussed above are exhibited.
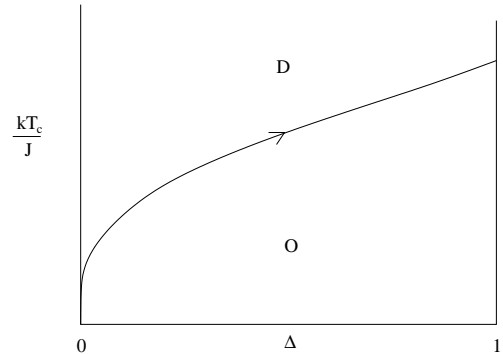

FIG. 1. Schematic plot of the temperature vs. anisotropy phase-diagram for the two-dimensional anisotropic ferromagnetic Heisenberg model, where O stands for the ferromagnetic (ordered) phase and D stands for the paramagnetic (disordered) phase. The arrow indicates that the transitions for $\Delta \ne 0$ belong to the same universality class as for the Ising model ($\Delta = 1$). Note that the critical temperature line goes to zero in the limit of the isotropic Heisenberg model ($\Delta = 0$).

For many classical (and some quantum) systems on bipartite lattices, there is a mapping of the ferromagnetic model onto the antiferromagnetic one. Neverthe-

less, there is no such mapping for the Heisenberg model; therefore, the ground state of the anisotropic antiferromagnetic Heisenberg (AAH) model is not obtained from its ferromagnetic couterpart by flipping all spins in a given sub-lattice. In fact, the ground state for $J < 0$ is not even exactly known and has been a matter of debate for a long time. However, long-range order was proven to be present at $T = 0$ for $\Delta > \Delta_c = 0.40$ [4], whereas the same authors, using extra assumptions, calculated a lower value of Δ_c, namely, $\Delta_c = 0.09$ [4].

Previous RSRG procedures have been able to calculate the approximate phase-diagram for the AAH on the square lattice [5,6]. The former reference uses a hierarchical lattice to approximate the square one, and performs a partial trace over internal degrees of freedom, in a manner introduced in Ref. [7]. This approach was the extension of the Niemeijer-van Leeuwen method to quantum spin systems. On the other hand, Ref. [6] applies the so-called mean-field renormalization group ideas. Although the approximate scaling transformations calculated in Refs. [5] and [6] are different, the results obtained are qualitatively the same, and we will comment on them when our results are discussed. Nevertheless, one should bear in mind that RSRG procedures on quantum systems do not have the same firm basis as on classical models. The reason is the non-commutivity aspects of the Hamiltonian and, in as concerns Ref. [6], the necessity of introducing symmetry-breaking fields which are chosen according to the ground state of the *classical* Ising model.

Results from spin-wave theory [8] on the isotropic Heisenberg model give the same value for the critical temperature of the ferromagnetic *and* antiferromagnetic systems [9], which is in direct contradiction to rigorous results [10] and to some approximate calculations [5,6].

Therefore, the form of the phase-diagram of the AAH model on the square lattice is far from a settled question and more work is desirable to study its critical properties. We thus apply two different RSRG procedures to evaluate the approximate phase-diagram of this system. The ferromagnetic Heisenberg case was also studied, in order to compare our results with previous ones for a model for which the critical behavior is well known.

The remainder of this paper is organized as follows. In section II we outline the formalism we used, in section III we present results, and in the last section we summarize our main conclusions.

II. FORMALISM

In this section we outline the finite-size scaling RG (FSSRG) procedure, since it is somewhat new in the literature and, to the best of our knowledge, has never been used in the study of quantum systems. This method was proposed some time ago [11] and has been successfully applied to classical systems (both static and dynamic properties have been studied), like Ising, Potts, or Blume-Capel models [12]. The second is just the generalization of the usual bond-moving Migdal-Kadanoff [13] approximation to antiferromagnetic quantum systems.

The finite-size scaling assumption is that, near the critical region, thermodynamic quantities have the following form [14]:

$$\mathcal{F}(\varepsilon, L) = b^{\psi} \mathcal{F}\left(b^{1/\nu}\varepsilon, b^{-1}L\right), \quad (2)$$

where b is some arbitrary scaling factor, L is the linear dimension of the lattice, $\mathcal{F}$ is a scaling function, $\varepsilon \equiv |T - T_c|$ (T_c is the critical temperature), and ν is the critical exponent of the correlation length, such that $\xi \sim \varepsilon^{-\nu}$ for T close to T_c and in the thermodynamic limit. The exponent ψ is the anomalous dimension of the thermodynamic quantity $\mathcal{F}$; for the magnetization M, $\psi = -\beta/\nu$, while for the magnetic susceptibility χ, $\psi = \gamma/\nu$.

The idea behind the FSSRG is to construct quantities which have a zero anomalous dimension, $\psi = 0$, such that:

$$\mathcal{Q}_{L'}(\varepsilon') \equiv \mathcal{Q}_{L'}(b^{1/\nu}\varepsilon) = \mathcal{Q}_L(\varepsilon). \quad (3)$$

As seen, these quantities will have the same value at $T = T_c$, no matter what the lattice sizes L or L' are (as far as both are $\gg 1$). Therefore, the crossing of $\mathcal{Q}$ for two different lattice sizes is an evaluation of the critical temperature; furthemore, the previous equation can be seen as an iteration, in the renormalization group (RG) sense. Thus, information on the exponent ν can also be accessed, as well as other information obtained from RG procedures (universality classes, crossover phenomena, first order phase transitions, etc). For example, for the Ising model in zero magnetic field, one apropriate function is:

$$\tau = \left\langle \text{sign}\left(\sum_{top} S_t\right) \text{sign}\left(\sum_{bottom} S_b\right)\right\rangle \quad (4)$$

where $\langle \ldots \rangle$ denotes a canonical average, *bottom* means all spins at the bottom plane(line) of a three(two)-dimensional lattice, *top* stands for all spins at the top plane(line) of a three(two)-dimensional lattice, and $\text{sign}(x) = -1, 0$ or 1 if $x < 0$, $x = 0$ or $x > 0$, respectively. For an infinite system, $\tau = 1$ for $T < T_c$ and $\tau = 0$ for $T > T_c$. Replacing τ for $\mathcal{Q}$ in Eq. 3, we obtain a RSRG equation which connects the parameters K in the original lattice and K' in the renormalized (smaller) lattice. For a more detailed discussion on the application of the FSSRG to the Ising model, see Ref. [11]. Note, however, that the only approximation comes from the finite size of the lattices; in fact, even when small lattices are used, the quantitative results are precise, and

this can be understood if one realizes that the FSSRG is a generalization, for completely finite clusters, of the phenomenological RG developed by Nightingale [15].

In using the FSSRG approach in the study of quantum systems, we expect to take advantage of the fact that non-commutative aspects of the Hamiltonian are not approximated away by the method. Our approach here is to use small lattices, which, although not allowing for a precise evaluation of the critical parameters (like, for instance, those obtained with numerical simulations on big lattices), allows for a good qualitative description of the critical phenomena involved. The lattices we chose to represent the square lattice are depicted in Fig. 2, where the right figure is the bigger cluster, with parameters $K \equiv J/kT$ and Δ and the left figure depicts the smaller cluster, with parameters K' and Δ'. The Hamiltonian for the original and renormalized clusters are:

$$-\beta\mathcal{H} = K \left[(1 - \Delta)(S_1^x S_2^x + S_1^y S_2^y + S_2^x S_3^x + S_2^y S_3^y + \right.$$

$$S_3^x S_4^x + S_3^y S_4^y + + S_4^x S_1^x + S_4^y S_1^y) +$$

$$\left. S_1^z S_2^z + S_2^z S_3^z + S_3^z S_4^z + S_4^z S_1^z \right], \qquad (5)$$

and

$$-(\beta\mathcal{H})' = K' \left[(1 - \Delta') \left(S_1^x S_2^x + S_1^y S_2^y \right) + S_1^z S_2^z \right], \quad (6)$$
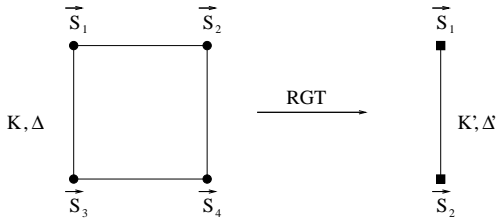
respectively.

FIG. 2. Cells used to implement the renormalization group transformation for the anisotropic Heisenberg model on the square lattice.

When applying the FSSRG method to the anisotropic Heisenberg model, one has to devise two functions with zero anomalous dimension, since it is necessary to renormalize two parameters, namely, Δ and kT/J. Also, we have to distinguish between the antiferromagnetic and ferromagnetic models, and two different sets of functions were used for each of them.

For the ferromagnetic model, we chose the following quantities:

$$\tau' = \langle \text{sign}(S_1^z)\text{sign}(S_2^z) \rangle \,; \qquad (7)$$

$$\eta' = \langle \text{sign}(S_1^x)\text{sign}(S_2^x) \rangle \qquad (8)$$

for the smaller cluster and

$$\tau = \langle \text{sign}(S_1^z + S_2^z)\text{sign}(S_3^z + S_4^z) \rangle \qquad (9)$$

$$\eta = \langle \text{sign}(S_1^x + S_2^x)\text{sign}(S_3^x + S_4^x) \rangle \qquad (10)$$

for the bigger cluster. The averages are to be taken with respect to the ensemble defined by Eq. 5 (6) for unprimed (primed) quantities.

For the antiferromagnetic model, Eqs. 7 and 8 remain the same, while Eqs. 9 and 10 are replaced by:

$$\tau = \langle \text{sign}(S_1^z - S_2^z)\text{sign}(-S_3^z + S_4^z) \rangle \qquad (11)$$

and

$$\eta = \langle \text{sign}(S_1^x - S_2^x)\text{sign}(-S_3^x + S_4^x) \rangle \,, \qquad (12)$$

respectively.

The procedure to calculate these functions is fairly straightforward; the final expressions, however, are too lengthy and will be omitted. To obtain the required RG equations, we impose $\tau' = \tau$ and $\eta' = \eta$, according to Eq. 3. Approximate values for the critical points are obtained from the fixed points of these equations and critical exponents are linked to the behavior of the iterations near the fixed points.

III. RESULTS

A. Finite-size scaling renormalization group (FSSRG)

Our results for the ferromagnetic (F) and antiferromagnetic (AF) models are shown in Fig. 3. The critical curve for the F curve is depicted for comparison: the accordance with previous results, either approximate or exact, is very good. The Ising critical point is located at $kT_c/|J| = 2.11, \Delta = 1$ (exact values: $kT_c/|J| = 2.269, \Delta = 1$); our estimate for the critical exponent ν for the Ising model is 0.91, while the exact value is 1. The universality class for $\Delta \neq 0$ is the same as for the Ising model, which is also consistent with previous results. Note that the F and AF Ising models are expected to have the same critical exponents and the same modulus of the critical temperature, and our evaluation agrees with these results.

For the AF model, the phase diagram is qualitatively different from its F counterpart: the critical temperature reaches zero at a critical value of Δ, Δ_c, which is greater than zero. We find $\Delta_c = 0.29$, which compares with $\Delta_c = 0.40$ in Ref. [5] and $\Delta_c = 0.18$ in Ref. [6]. We also find a reentrant behavior in the critical line, which is also present in Refs. [5,6]. Nevertheless, in Ref. [6] a second reentrance is observed; the lowest temperature we could work with was $kT/|J| = 0.1$ and we have observed no sign of this second reentrance, neither with the FSSRG nor with the bond-moving scheme

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(to be presented in what follows). In Ref. [6], the Néel temperature behaves as $T_N \sim 1/\log(\Delta - \Delta_c)$ near $\Delta = \Delta_c$, while, for the anisotropic ferromagnetic Heisenberg model, $T_c \sim 1/\log(\Delta)$ [6]. The supression of long-range order at finite temperatures for small values of Δ can be regarded as due to quantum fluctuations. While these are not relevant in critical phenomena which take place at "high" temperatures, they might be important when the critical temperature is low. We expect this to be the case for small values of Δ, and then quantum fluctuations gain in importance, supressing long-range order. Note that we cannot present results at $T = 0$, since parts of our calculation were done numerically and, therefore, we are not able to go to very low temperatures.
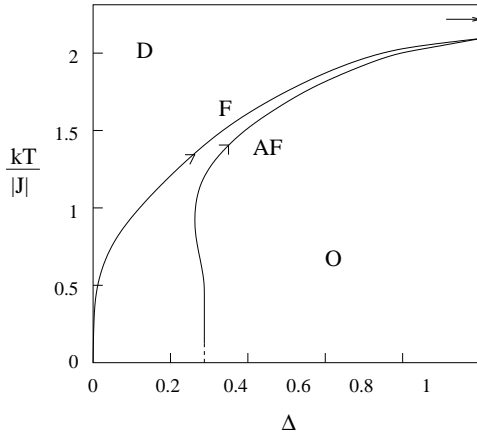

FIG. 3. Critical temperature vs. anisotropy phase-diagram for the ferromagnetic (curve F) and anti-ferromagnetic (curve AF) anisotropic Heisenberg model. Both lines are atracted to the Ising fixed-point, located at $kT/|J| = 2.11$, $\Delta = 1$. $O(D)$ stands for ordered (disordered) phase. The arrow indicates the exact critical temperature for the Ising model.

B. Migdal-Kadanoff approximation

We have also performed a bond-moving RSRG procedure to study the AAH model on the square lattice. This procedure is equivalent to the one in Ref. [5] applied to a different hierarchical lattice; a careful exposition of the method is made in Ref. [7] and the bond-moving approximation is presented in Ref. [16].

The phase-diagram for the antiferromagnetic model is presented in Fig. 4; note that the qualitative features agree with those obtained from other RSRG approaches. However, we have not found the second reentrance in the critical curve. The Néel temperature T_N varies as (see insert in Fig. 4):

$$T_N \sim \frac{1}{\log(\Delta_c - \Delta)}, \qquad (13)$$

where $\Delta_c = 0.199$ for the Migdal-Kadanoff approximation. Again the universality class for the whole critical curve is the same as for the Ising model.
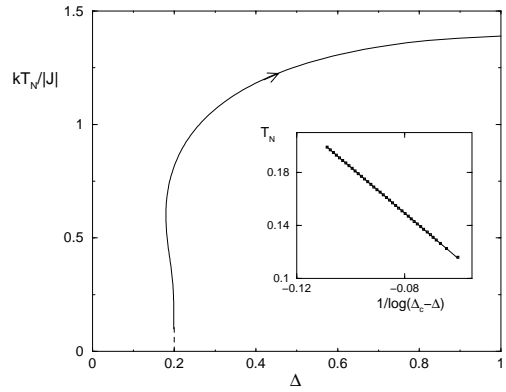

FIG. 4. Néel temperature T_N vs. Δ phase-diagram for the antiferromagnetic anisotropic Heisenberg model on the square lattice. The region above (below) the critical line represents a(n) desordered (ordered) phase and the insert shows the data for small T_N, near $\Delta_c = 0.199$.

We would like to mention that the results from both RSRG employed here are in disagreement with spin-wave calculations [8,9] and numerical simulation [17,18]. The former presents $T_c = T_N$ for any value of Δ and for two and three dimensions, while the latter predicts $\Delta_c = 0$ for the AAH model. In Ref. [18], the logarithmic dependence of T_N and T_c with respect to $\Delta - \Delta_c$ is established using scaling arguments, but $\Delta_c = 0$ in that paper. Note that our calculations cannot be carried out down to $T = 0$; therefore, we cannot study the character of the ground state of the AAH model [4,19].

IV. SUMMARY

In summary, we calculate the $kT/|J|$ vs. Δ phase-diagram for the anisotropic antiferromagnetic Heisenberg model on the square lattice. Our results show the presence of reentrant behavior on the critical line which separates the disordered and ordered phases and a value of $\Delta > 0$ such that the Néel temperature is zero. The entire critical line is found to belong to the universality class of the Ising model. These findings are in agreement with previous RSRG procedures (with the exception of the second reentrance found in Ref. [6]) but not with spin-wave calculations and numerical simulation.

It is clear that the reentrant behavior and a value of Δ_c greater than zero are strongly supported by RSRG approaches, but the question is not yet settled and more work is needed to put these points on firmer grounds. Coherent-anomaly methods [20] and numerical simulations with cluster algorithms [21] are possible ways to provide a more definite answer to this problem. Work is now proceeding along these lines.

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